

Migration and Chemical Reaction of H⁺ in Protonated β-D-Galactose

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Supporting Information

Table. The energies and chemical potentials of conformers and transitions states.

	B3LYP/6-31G(d)		B3LYP/6-311++G(d,p)			
	E (a.u.)	ΔE (kcal/mol)	E (a.u.)	ΔE (kcal/mol)	CP (298.15K) (kcal/mol)	CP (40K) (kcal/mol)
1	-687.149721	0.00	-687.3984371	0.00	48.99	9.84
2	-687.1417334	5.01	-687.3899523	5.32	49.56	10.09
3	-687.1388511	6.82	-687.3887306	6.09	49.56	9.87
TS1-2	-687.1373019	7.79	-687.3859429	7.84	48.79	10.07
TS1-3	-687.1335142	10.17	-687.3853008	8.24	48.31	9.50
TS2-3	-687.1375441	7.64	-687.3860057	7.80	48.03	9.67

Geometries of conformers and transition states

1

B3LYP/6-31G(d)

C	-1.3107574612	1.0000571246	0.3543663374
C	-1.5925239120	-0.2749735908	-0.4800243660
C	-0.3642632040	-1.1756471668	-0.7014611984
C	0.4881806531	-1.2969206491	0.5663697078
C	0.7833236020	0.0787222913	1.2169576545
O	-0.4315127630	0.8176086912	1.4277958954
O	-2.4719012807	-1.1030588483	0.2628251836
O	0.4461379491	-0.6840139928	-1.8048163701
C	1.8764847925	0.9159417813	0.5484645804
O	1.5415989983	1.3369804157	-0.8326500981

H	-3.3843894957	-0.7888921441	0.1614369565
H	1.2413959256	0.4860281578	-1.3737148181
H	0.6550086667	1.8624756727	-0.7887377234
H	-2.0059713154	0.0220791257	-1.4518688572
H	-0.7395707372	-2.1606503317	-0.9885498841
H	1.1614195693	-0.1032740881	2.2295534991
H	2.0458841041	1.8439759629	1.0954217214
H	2.8054965246	0.3534707624	0.4648517463
O	-0.8597784078	2.0579957937	-0.5341279973
H	-2.2463323736	1.3311161375	0.8103752009
H	-0.0860659901	-1.8837247875	1.2912287181
O	1.7047441980	-1.9334235026	0.1929624275
H	1.9192208877	-2.6428674145	0.8179124296
H	-1.0522940541	2.9186837781	-0.1210767586
H	1.0712042259	-1.3995150644	-2.0283214997

B3LYP/6-311++G(d,p)

C	-1.3044479588	1.0036980284	0.3595260552
C	-1.5884779945	-0.2788561832	-0.4621543047
C	-0.3534957723	-1.1686475523	-0.6940679169
C	0.4920426512	-1.2915359054	0.5770773759
C	0.7953873095	0.0832618011	1.2208131711
O	-0.4199703119	0.8246211776	1.4287296786
O	-2.4648872756	-1.1073552506	0.2865058402
O	0.4487493801	-0.6473525931	-1.7911958258
C	1.8935434629	0.9154429273	0.5588184321
O	1.5590176532	1.3451040094	-0.8219781296
H	-3.3827206647	-0.8509524862	0.1434614809
H	1.2539502269	0.5084322524	-1.3651809191
H	0.6952576962	1.8832766365	-0.7821309566
H	-2.0116090110	0.0100474547	-1.4284712558
H	-0.7178107356	-2.1521495287	-0.9911767765
H	1.1676856339	-0.1003154641	2.2329370039
H	2.0670554782	1.8366973467	1.1114180994
H	2.8169419076	0.3475989725	0.4736341465
O	-0.8428165509	2.0507551753	-0.5368168064
H	-2.2349318899	1.3403662172	0.8163371366
H	-0.0945804604	-1.8637096222	1.3002611655
O	1.7091775703	-1.9466759388	0.2414740679
H	1.8563876351	-2.7100582620	0.8096974482
H	-1.1446443800	2.9124160817	-0.2198874418
H	0.9999355025	-1.3659351800	-2.1324582814

2

B3LYP/6-31G(d)

C	1.2148128864	-1.0515853099	0.3898355235
C	1.8203843619	0.1812941735	-0.3065272795
C	0.6789659694	1.0363839581	-0.8611823824
C	-0.3653840722	1.3644386299	0.2285954495
C	-0.7201248966	0.2020052623	1.2125651941
O	0.3433189513	-0.7777975505	1.3927497588
O	2.4831319913	0.9717818109	0.6516865010
O	0.0719460556	0.2913042566	-1.9335413558
C	-2.0277013812	-0.5568159720	0.9856048418
O	-1.9337291752	-1.3852790953	-0.1920248660
H	3.3891776582	0.6510223383	0.7864283582
H	-0.8538573752	0.6075664254	-2.0011062128
H	-2.7422042395	-1.9173375902	-0.2769579502
H	2.4748369105	-0.1408296921	-1.1277727717
H	1.0868853856	1.9707806117	-1.2618473645
H	-0.8207962127	0.6483232894	2.2055457128
H	-2.2020349205	-1.1866212320	1.8650854240
H	-2.8463105489	0.1584288679	0.8743450228
O	0.4963821747	-1.8628798009	-0.7315492277
H	1.9518886821	-1.7556696564	0.7746959702
H	0.0507002476	2.1771508888	0.8315004584
O	-1.5712434429	1.7667847268	-0.4194194985
H	-1.5765337889	2.7315265928	-0.5288610846
H	-0.4487982858	-2.0410366730	-0.3891685732
H	0.2856489951	-1.1624105358	-1.4666244287

B3LYP/6-311++G(d,p)

C	1.2072450224	-1.0513823325	0.3938275148
C	1.8161025376	0.1771174535	-0.3041924616
C	0.6819453394	1.0372941212	-0.8638694044
C	-0.3643157681	1.3637746077	0.2204842668
C	-0.7323715074	0.2017619941	1.2020194472
O	0.3328034901	-0.7775418828	1.3899955596
O	2.4937951881	0.9612387536	0.6506395565
O	0.1026776689	0.2905218093	-1.9497189557
C	-2.0420698344	-0.5558389753	0.9871366008
O	-1.9318995420	-1.4704411466	-0.1273299060
H	3.4083862386	0.6744426455	0.7522351381
H	-0.7672333696	0.6698821897	-2.1544622835
H	-2.7403596669	-1.9902027230	-0.2118632205
H	2.4674020583	-0.1482155041	-1.1225262268
H	1.0936966536	1.9716290678	-1.2528867090

H	-0.8317500899	0.6543510466	2.1901373429
H	-2.2478061643	-1.1254678876	1.8966339012
H	-2.8462327968	0.1568378321	0.8018553157
O	0.4878027468	-1.8636121637	-0.7323078594
H	1.9418733691	-1.7554823770	0.7776667832
H	0.0646798595	2.1619028122	0.8293507787
O	-1.5535342141	1.8058637310	-0.4303457965
H	-1.6413245268	2.7632304141	-0.3657280920
H	-0.4558028408	-2.0419813418	-0.4005442723
H	0.2956520787	-1.1891534196	-1.4741517984

3

B3LYP/6-31G(d)

C	-1.1836975740	1.2326894956	-0.0316300846
C	-1.7698511026	-0.1702097677	-0.2901210137
C	-0.5995596387	-1.1500386778	-0.4624261460
C	0.2530008907	-1.1722457434	0.8080696750
C	0.7427969845	0.2442017026	1.2228206535
O	-0.2270911768	1.2901492884	0.9774903386
O	-2.4903819404	-0.6543770717	0.8190020601
O	0.2300449177	-0.6932246098	-1.6265240968
C	2.1350752655	0.6129448485	0.7085136814
O	2.2241630560	0.4926468469	-0.7332405644
H	-3.3988788808	-0.3137055308	0.7965359398
H	1.2054153751	-0.5290403222	-1.3154218380
H	3.1577783604	0.4284736622	-0.9946629632
H	-2.3776909450	-0.1343885999	-1.2040781705
H	-0.9418463090	-2.1490177537	-0.7332180710
H	0.8461466357	0.2456634698	2.3125899673
H	2.3493668607	1.6484580240	0.9927570564
H	2.8594363085	-0.0554994261	1.1794909407
O	-0.6644248696	1.6258129385	-1.3275449516
H	-1.9570987933	1.9453253731	0.2677357764
H	-0.4089680786	-1.5465079307	1.5960535251
O	1.4006327386	-1.9865184169	0.6414799384
H	1.1828116808	-2.9066089304	0.8608094984
H	-0.1259834591	2.4321390145	-1.2337543021
H	-0.0570944113	0.2799703973	-1.8191977717

B3LYP/6-311++G(d,p)

C	-1.1907011946	1.2464280283	-0.0096597917
C	-1.7535086913	-0.1612162928	-0.2926167198
C	-0.5731409409	-1.1245979146	-0.4824369653

C	0.2569448343	-1.1640563993	0.7995207818
C	0.7592708139	0.2443437763	1.2161111055
O	-0.2118438624	1.2934876185	0.9863554132
O	-2.4820120446	-0.6728658139	0.8017852057
O	0.2635649261	-0.6405490010	-1.6280121964
C	2.1538960353	0.5995824259	0.7004043437
O	2.2913430297	0.3706929011	-0.7350127726
H	-3.4049110492	-0.3989894230	0.7545137954
H	1.2456530039	-0.3807516060	-1.2964143444
H	3.2013935943	0.1370881586	-0.9559888307
H	-2.3601435148	-0.1162262081	-1.2029431286
H	-0.9052844408	-2.1191262657	-0.7727678499
H	0.8690133745	0.2419409939	2.3034407674
H	2.3512307880	1.6536934189	0.8998521521
H	2.8789729967	-0.0237443855	1.2221257706
O	-0.7055099706	1.6819816547	-1.2938352711
H	-1.9741607951	1.9246097611	0.3328190431
H	-0.4252402109	-1.5224477384	1.5733403205
O	1.3889056533	-2.0098355746	0.6701160869
H	1.1828775867	-2.8991911132	0.9784298506
H	-0.3921912462	2.5953897182	-1.2603411692
H	-0.0803167802	0.2614515609	-1.8972565192

TS1-2

B3LYP/6-31G(d)

C	1.1042488346	-1.2325952721	0.2005423518
C	1.8087523306	0.0393289882	-0.3021657959
C	0.7616002405	1.0852850857	-0.6815002449
C	-0.2449129938	1.3214381790	0.4673421548
C	-0.6899666296	0.0476593565	1.2641207577
O	0.2740143826	-1.0519922906	1.2467559507
O	2.5494279177	0.5851268267	0.7659163363
O	0.1122694561	0.6061734389	-1.8676545626
C	-2.0430090915	-0.5443867527	0.8749259287
O	-2.0546208412	-1.0259432761	-0.4869455130
H	3.4117167369	0.1454600428	0.8406087286
H	-2.1453846854	-0.2520616089	-1.0729305120
H	-0.7465599517	-1.6677632110	-0.7875160243
H	2.4294751352	-0.1914331529	-1.1787752919
H	1.2708177904	2.0302383574	-0.8970058522
H	-0.7475629844	0.3078260865	2.3251360310
H	-2.2431865160	-1.4164961257	1.5003853353
H	-2.8447628755	0.1838999302	1.0084032423

O	0.2790085719	-1.8304446326	-1.0129026619
H	1.7777139541	-2.0544886660	0.4402325503
H	0.2472398659	1.9945218422	1.1755689318
O	-1.3780795144	1.9460955926	-0.1386946656
H	-1.6825642857	2.6894852213	0.4045350065
H	0.3953623599	-1.2264479784	-1.7904861710
H	-0.4250369895	1.3280825084	-2.2347646528

B3LYP/6-311++G(d,p)

C	1.1094662473	-1.2175914814	0.2022698054
C	1.8072636410	0.0566011944	-0.3006955259
C	0.7586886474	1.1082023955	-0.6630715057
C	-0.2230701793	1.3316330953	0.5029459931
C	-0.7160031602	0.0436117738	1.2350012500
O	0.2597049232	-1.0461892290	1.2346399174
O	2.5760286630	0.5881537268	0.7570829221
O	0.1006327360	0.6381174541	-1.8464740855
C	-2.0658870435	-0.5482536252	0.8332443740
O	-2.0362305819	-1.1945834648	-0.4657666278
H	3.4592970003	0.2023087381	0.7757372641
H	-2.4225092581	-0.6184538329	-1.1368558611
H	-0.7194364526	-1.6938252348	-0.8012019428
H	2.4153591537	-0.1715788220	-1.1831480044
H	1.2689243116	2.0516472993	-0.8738314352
H	-0.8106161439	0.2901473810	2.2947531878
H	-2.3258819628	-1.3294627166	1.5473180504
H	-2.8362839288	0.2205453550	0.8395725779
O	0.3091752072	-1.8283389053	-1.0161405902
H	1.7907246852	-2.0260901219	0.4560237007
H	0.3122295337	1.9309131242	1.2424112578
O	-1.3506647979	2.0410779640	-0.0081823913
H	-1.4453883542	2.8941336547	0.4288218067
H	0.4261322634	-1.2449052530	-1.7978282296
H	-0.4656549321	1.3387480201	-2.1934945502

B3LYP-D/TZVP

C	1.1042488346	-1.2325952721	0.2005423518
C	1.8087523306	0.0393289882	-0.3021657959
C	0.7616002405	1.0852850857	-0.6815002449
C	-0.2449129938	1.3214381790	0.4673421548
C	-0.6899666296	0.0476593565	1.2641207577
O	0.2740143826	-1.0519922906	1.2467559507
O	2.5494279177	0.5851268267	0.7659163363
O	0.1122694561	0.6061734389	-1.8676545626

C	-2.0430090915	-0.5443867527	0.8749259287
O	-2.0546208412	-1.0259432761	-0.4869455130
H	3.4117167369	0.1454600428	0.8406087286
H	-2.1453846854	-0.2520616089	-1.0729305120
H	-0.7465599517	-1.6677632110	-0.7875160243
H	2.4294751352	-0.1914331529	-1.1787752919
H	1.2708177904	2.0302383574	-0.8970058522
H	-0.7475629844	0.3078260865	2.3251360310
H	-2.2431865160	-1.4164961257	1.5003853353
H	-2.8447628755	0.1838999302	1.0084032423
O	0.2790085719	-1.8304446326	-1.0129026619
H	1.7777139541	-2.0544886660	0.4402325503
H	0.2472398659	1.9945218422	1.1755689318
O	-1.3780795144	1.9460955926	-0.1386946656
H	-1.6825642857	2.6894852213	0.4045350065
H	0.3953623599	-1.2264479784	-1.7904861710
H	-0.4250369895	1.3280825084	-2.2347646528

TS2-3

B3LYP/6-31G(d)

C	1.2607890233	-1.0739448571	0.4093733817
C	1.8233738669	0.1685809259	-0.3093219923
C	0.6348041930	0.9737778726	-0.8451128105
C	-0.3519852525	1.3476985653	0.2679212551
C	-0.7175143491	0.1700466622	1.2242162785
O	0.3564228629	-0.7869113268	1.4112670424
O	2.4696834482	1.0395359222	0.5867959070
O	-0.0770848022	0.1169531871	-1.8330173965
C	-2.0305869457	-0.5500079838	0.9177907653
O	-1.9787758021	-1.1647103268	-0.3809622880
H	3.3719383572	0.7274136575	0.7622632012
H	-1.0490882489	0.2798555436	-1.7144374416
H	-2.8492944846	-1.5512974409	-0.5705153868
H	2.4693730551	-0.1533047492	-1.1377017680
H	0.9616762588	1.8567251956	-1.3961887893
H	-0.8503540603	0.5963623010	2.2227912816
H	-2.1814071171	-1.3100291068	1.6940988189
H	-2.8444859944	0.1796534911	0.9665361561
O	0.6652933465	-1.8753342641	-0.6780975699
H	2.0403231824	-1.6822526401	0.8728064690
H	0.1241990291	2.1355856958	0.8596756515
O	-1.5587105078	1.7969213489	-0.3423954274
H	-1.5090509620	2.7528257266	-0.5077178849

H	-0.0786801802	-2.3929900620	-0.3087010243
H	0.1182782113	-0.9132314595	-1.4813718971

B3LYP/6-311++G(d,p)

C	1.2544912850	-1.0711948592	0.4101496169
C	1.8217422425	0.1725646306	-0.3015176534
C	0.6363449106	0.9722714906	-0.8497415838
C	-0.3536712377	1.3451015378	0.2576607132
C	-0.7293131155	0.1725560054	1.2162504427
O	0.3406259301	-0.7992222950	1.3976004765
O	2.4705401027	1.0332323285	0.6037127528
O	-0.0410994260	0.1056868566	-1.8407432871
C	-2.0476528260	-0.5404787411	0.9335967911
O	-2.0077295870	-1.2023002381	-0.3429123160
H	3.3855349897	0.7628520223	0.7419189694
H	-0.9985827673	0.3134029255	-1.8354668376
H	-2.8735597452	-1.5861151162	-0.5243827386
H	2.4741950681	-0.1465774890	-1.1214795567
H	0.9680776620	1.8588372643	-1.3882013003
H	-0.8441520844	0.6019882436	2.2133520969
H	-2.2064185991	-1.2705634450	1.7328004951
H	-2.8507460683	0.1991851746	0.9547130746
O	0.6597238430	-1.8612638511	-0.7045973876
H	2.0254330602	-1.6942227368	0.8618958183
H	0.1247841739	2.1260560650	0.8520936777
O	-1.5491502179	1.8185790024	-0.3581725819
H	-1.5438588373	2.7809152075	-0.4181147503
H	-0.0336807904	-2.4465165220	-0.3555911104
H	0.1372581619	-0.9568515829	-1.4448292899

B3LYP-D/TZVP

C	1.25449133	-1.07119489	0.41014960
C	1.82174230	0.17256463	-0.30151767
C	0.63634491	0.97227150	-0.84974158
C	-0.35367122	1.34510159	0.25766072
C	-0.72931314	0.17255600	1.21625042
O	0.34062594	-0.79922229	1.39760053
O	2.47054005	1.03323233	0.60371274
O	-0.04109943	0.10568686	-1.84074330
C	-2.04765272	-0.54047877	0.93359679
O	-2.00772953	-1.20230019	-0.34291232
H	3.38553500	0.76285201	0.74191898
H	-0.99858278	0.31340292	-1.83546686
H	-2.87355971	-1.58611512	-0.52438277

H	2.47419500	-0.14657749	-1.12147951
H	0.96807766	1.85883725	-1.38820136
H	-0.84415209	0.60198826	2.21335220
H	-2.20641851	-1.27056348	1.73280048
H	-2.85074615	0.19918518	0.95471305
O	0.65972382	-1.86126387	-0.70459741
H	2.02543306	-1.69422269	0.86189580
H	0.12478418	2.12605596	0.85209370
O	-1.54915023	1.81857896	-0.35817257
H	-1.54385889	2.78091526	-0.41811475
H	-0.03368079	-2.44651651	-0.35559112
H	0.13725816	-0.95685160	-1.44482934

TS1-3

B3LYP/6-31G(d)

C	-1.1840367616	1.2410622114	-0.0246589109
C	-1.7566789596	-0.1648281067	-0.3004072694
C	-0.5880964861	-1.1449996984	-0.4687865917
C	0.2514009677	-1.1659620830	0.8113298112
C	0.7379518066	0.2504923339	1.2240151499
O	-0.2408883517	1.2881188681	1.0041028204
O	-2.4902925394	-0.6604811648	0.7961154382
O	0.2532294200	-0.7075044797	-1.6322394479
C	2.1247764079	0.6150098336	0.6851829308
O	2.2713748896	0.3717260260	-0.7466177013
H	-3.3971485754	-0.3159546680	0.7688393344
H	1.2305725076	-0.3651334980	-1.2904252806
H	2.5044840347	1.1869416151	-1.2183871814
H	-2.3582129996	-0.1229220325	-1.2187869130
H	-0.9339301278	-2.1441468420	-0.7352217538
H	0.8645265098	0.2443580378	2.3117838046
H	2.3225949062	1.6689822044	0.8936705234
H	2.8727243014	-0.0049079337	1.1800422083
O	-0.6580409401	1.6681430729	-1.2934561700
H	-1.9766538624	1.9257690638	0.2914536181
H	-0.4268348449	-1.5303807348	1.5906171470
O	1.4014456293	-1.9773825869	0.6779657168
H	1.1756999305	-2.9028957133	0.8637683779
H	-0.4892182885	2.6248525817	-1.2876255315
H	-0.1302707842	0.1456398728	-1.9801355296

B3LYP/6-311++G(d,p)

C	1.3810210751	-1.0065862390	0.4264581843
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C	1.7620174041	0.2576855878	-0.3699105008
C	0.4825314870	0.9338702129	-0.8815519001
C	-0.4056827088	1.3050722394	0.3075306181
C	-0.7168659044	0.0879679682	1.2200770997
O	0.4159947479	-0.7831887175	1.4160683009
O	2.3863645997	1.2314067701	0.4378498760
O	-0.2463662090	0.0031102892	-1.7989497764
C	-1.9993883468	-0.6632474290	0.8604784223
O	-2.0893535706	-0.9592574470	-0.5695244690
H	3.3270043428	1.0438611610	0.5328892856
H	-1.1516425454	-0.4246206627	-1.3133614892
H	-2.4169348505	-1.8482524170	-0.7482426227
H	2.3980415283	-0.0415630634	-1.2109846388
H	0.7108842219	1.8079840468	-1.4884952501
H	-0.9099995385	0.4800956703	2.2219162839
H	-2.0313423514	-1.5981729704	1.4195096717
H	-2.8597699851	-0.0433624786	1.1067167984
O	0.9595263373	-1.9548922865	-0.5628229972
H	2.2463838592	-1.3951096405	0.9670323422
H	0.1851395472	2.0155953061	0.8902600573
O	-1.6427443177	1.8560935987	-0.1040354843
H	-1.5864342984	2.8163068479	-0.1621397358
H	1.0337699202	-2.8556059995	-0.2258817656
H	0.3091384360	-0.7893905330	-1.9541159505

B3LYP-D/TZVP

C	-1.2294847	1.2407616	-0.0314043
C	-1.7973390	-0.1578987	-0.3408093
C	-0.6384076	-1.1445917	-0.5064880
C	0.1981180	-1.1685070	0.7709674
C	0.6831001	0.2409527	1.1936841
O	-0.3208341	1.2601490	1.0293526
O	-2.5654207	-0.6683994	0.7249124
O	0.2015935	-0.7307562	-1.6714340
C	2.0467444	0.6370456	0.6344069
O	2.1667565	0.3737209	-0.7992273
H	-3.4553842	-0.2981952	0.7024031
H	1.1667969	-0.2900835	-1.3327087
H	2.5772091	1.1068614	-1.2740246
H	-2.3758308	-0.0965529	-1.2690430
H	-0.9995730	-2.1398397	-0.7525019
H	0.8410229	0.2087664	2.2728557
H	2.2038844	1.6996033	0.8153366
H	2.8151675	0.0447965	1.1266899

O	-0.6578208	1.6934859	-1.2656326
H	-2.0308849	1.9143045	0.2762874
H	-0.4829257	-1.5264665	1.5454566
O	1.3409059	-1.9921823	0.6438440
H	1.1260636	-2.9000958	0.8864628
H	-0.5869763	2.6553122	-1.2715977
H	-0.2264810	0.0378088	-2.1077882